

## CLAIMS

1. A method of identifying a compound that modulates intermolecular interactions between a target protein and a modifier comprising the steps of:
- a) identifying a cavity on said target protein proximal to a
- 5 functionally critical site of said target protein that is involved in intermolecular interactions with said modifier;
- b) calculating dimensions of said cavity and mapping chemical and/or electrostatic properties of said cavity;
  - c) identifying compounds that contain functional groups that can be
- 10 accommodated by said cavity;
- d) testing said compounds in an *in vitro* assay to detect a compound which modulate intermolecular interactions between said target protein and said modifier.
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2. A pharmaceutical composition comprising:
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- a) a pharmaceutically acceptable carrier or diluent; and
  - b) a therapeutically effective amount of a compound having a structure selected from the group consisting of Formulae I-XIX.
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3. A method of treating an individual suffering from an inflammatory condition comprising the step of administering to said individual a therapeutically
- 20 effective amount of a compound having a structure selected form the group consisting of Formulae I-III.
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4. A method of treating an individual suffering from an undesirable immune response or immunological condition comprising the step of administering to said individual a therapeutically effective amount of a compound having a structure selected
- 25 form the group consisting of Formulae I-VI.
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5. A method of treating an individual suffering from a bacterial infection comprising the step of administering to said individual
- a) penicillin or a penicillin derivative antibiotic, and

- 83 -

- b) a compound having a formula selected from the group consisting of Formulae VII-XIX.

T02T20-2490260